Quantum computation with ultracold atoms in a driven optical lattice

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(Dated: January 18, 2013)

We propose a scheme for quantum computation in optical lattices. The qubits are encoded in the spacial wavefunction of the atoms such that spin decoherence does not influence the computation. Quantum operations are steered by shaking the lattice while qubit addressability can be provided with experimentally available techniques of changing the lattice with single-site resolution. Numerical calculations show possible fidelities above 99% with gate times on the order of milliseconds.

In the last years tremendous progress has been made in controlling and observing ultracold atoms in optical lattice (OL) potentials [1]. One of the latest developments has been the optical detection of atoms with single-site resolution in lattices of increasingly smaller periodicity [2–5]. This technological advancement allowed, e.g., for a direct observation of the superfluid to Mott-insulator transition [6]. Along with these detection schemes comes the possibility to control the lattice potential with single-site resolution. Lately, this has been used to manipulate the spin of single atoms in an OL [7].

One of the possibly most important applications of these techniques is the implementation of a quantum computer that would dramatically improve the computational power for particular tasks. Compared to other possible candidate systems for the implementation of a quantum computer, neutral atoms in OLs have the advantage of a natural scalability to a large number of atoms encoding qubits and a weak coupling to the environment leading to long decoherence times [8]. Single-site addressability of large qubit systems may be one of the last milestones on the way to an OL quantum computer.

Many schemes proposed for quantum computation in OLs rely on encoding the qubits by atomic spin states [9–12]. Although single-qubit operations [2] and collective two-qubit operations [13] have been demonstrated, spin qubit states are generally disturbed by external magnetic fields that lead to their decoherence. This source of decoherence can be avoided by encoding the qubits in the spacial wave function of the ground and first excited state of Bosonic atoms localized at single sites of an OL [12, 14, 15]. In this Letter we show that a periodic modulation of the lattice position, i.e. a *shaking* of the lattice suffices to perform all quantum operations needed for quantum computation. The shaking of the OL can be studied in the context of Floquet theory showing that it effectively changes the hopping parameter of the system [16]. This effect has been verified experimentally, while revealing that the shaking also drives transitions from the first to the second Bloch band [17]. Qubit addressability is provided by manipulating the OL with single-site resolution. This enables the selective change of the energy spacing of specific sites and the driving of local transitions. Additional z rotations induced by

the lattice manipulation can be cancelled by refocusing schemes known from NMR quantum control [18].

In the following we consider a one-dimensional (1d) OL in x direction with a potential $V_L = V_0 \sin^2(kx)$ assuming tight confinement in the transversal directions. Lengths are given in units of $1/k$ and energies in units of the recoil energy $E_r = \hbar^2 k^2/(2m)$. In this system of units the lattice spacing is given as $d = \pi$ and the oscillator energy of the harmonic approximation of a single lattice site as $\hbar\omega_L = 2\sqrt{V_0}$. Ultracold Bosons in OLs are regularly described by the Bose-Hubbard model which uses the Wannier basis of the first Bloch band to formulate the Hamiltonian in second quantization [19]. In order to consider excitations to higher Bloch bands the basis has to be extended to include Wannier functions $w_{i,b}(x)$ of sites $i = 1 \ldots N$ and several bands $b = 1 \ldots n$. Generally, atoms in different Bloch bands are coupled by the interaction $V_{\text{int}}(x_1, x_2) = g\delta(x_1 - x_2)$. By means of a Feshbach resonance or strong transversal confinement one can make g sufficiently large to form a Mott insulator state in the first two Bloch bands with one atom per site. A lattice with unit filling then realizes a quantum register with $|0\rangle$ encoded by an atom in the excited state, and $|1\rangle$ encoded by one in the ground state [see Fig. 1 a)]. In the following

$$\left\| \begin{matrix} n_{2,1} & n_{2,2} & n_{2,3} & \cdots \\ n_{1,1} & n_{1,2} & n_{1,3} & \cdots \end{matrix} \right\rangle \tag{1}$$

shall denote a Fock state in the extended Wannier basis with occupation number $n_{i,j}$ of band i and site j. If the coupling between the bands and sites is small and no avoided crossing appears all important eigenstates can be characterized by their dominantly contributing Fock state. In this notation the qubits state $|001\rangle$ is encoded by the eigenstate with maximal overlap to $\left\| \begin{smallmatrix} 110 \\ 001 \end{smallmatrix} \right\rangle$.

In the co-moving frame of the lattice a shaking is described by $V_{\text{sh}} = f_{\text{sh}} x \cos(\omega_{\text{sh}} t - \varphi)$, where ω_{sh} is the frequency, φ the phase, and $f_{\text{sh}}(t)$ the force amplitude of shaking [20]. This perturbation leads to a coupling between Bloch bands with symmetric and antisymmetric Wannier functions [see Fig. 1 b)]. We note in passing that transitions between the ground and excited states can also be achieved by Raman transitions [21]. By means of $\hat{V}_{\text{sh}}$ one is generally able to drive transitions between
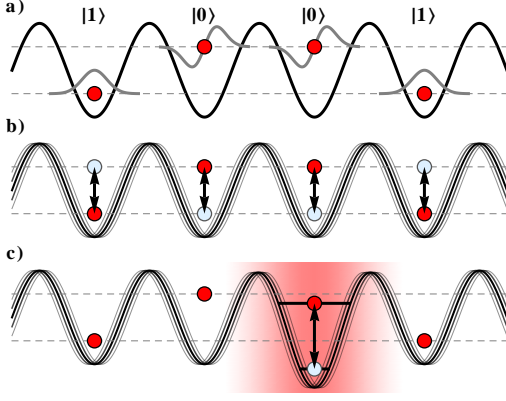
FIG. 1. (Color online) **a)** Qubit register with atoms (circles) in the ground ($\left\|{}^0_1\right\rangle = |1\rangle$) or excited state ($\left\|{}^1_0\right\rangle = |0\rangle$) of each lattice site. **b)** Shaking of the lattice couples predominantly ground and excited states in each lattice site (indicated by arrows). **c)** By shining a laser with waist on the order of the lattice spacing (red shading) onto one site a local transition between $|0\rangle$ and $|1\rangle$ can be driven by shaking the lattice.

different eigenstates of the lattice Hamiltonian $\hat{H}_0$. For this consider a Hamiltonian $\hat{\mathcal{H}}(t) = \hat{H}_0 + \lambda \hat{V} \cos(\omega t - \varphi)$, where $\hat{H}_0$ has two eigenstates $|\psi_1\rangle$, $|\psi_2\rangle$ with eigenenergies $\hbar\omega_1$ and $\hbar\omega_2$, respectively. For $\omega = \omega_2 - \omega_1$ the full time evolution operator in the rotating frame is given in terms of the Pauli matrices (σ_x, σ_y) as

$$\hat{U}(t) = \exp\left(\frac{i\Omega_R t}{2}\left[\cos(\varphi)\hat{\sigma}_x - \sin(\varphi)\hat{\sigma}_y\right]\right) \quad (2)$$

where $\Omega_R = \lambda|\langle\psi_1|\hat{V}|\psi_2\rangle|/\hbar$ is the Rabi frequency [22]. This enables arbitrary rotations about any axis in the xy plane of the system's Bloch sphere. A z rotation may be driven by combining rotations about the x and y axes.

Driving a single-qubit operation at a certain lattice site necessitates that the energy difference between $|0\rangle$ and $|1\rangle$ differs from that of other lattice sites. This can be achieved by shining a laser with a waist on the order of the lattice spacing perpendicular to the lattice, as was accomplished experimentally in [7]. The perturbation by this laser can be assumed to have the Gaussian form $V_{\text{Gauss}} = -\gamma \exp[(x - x_0)^2/(2\sigma^2)]$. Depending on whether the atoms are strong or weak-field seekers one has $\gamma > 0$ or $\gamma < 0$ and the additional intensity will enlarge or reduce the energy difference $\hbar(\omega_2 - \omega_1)$ between ground and excited state [see Fig. 1 c)]. By shaking with a frequency $\omega_{\text{sh}} = \omega_2 - \omega_1$ one is then able to drive single-qubit rotations on the marked lattice site.

The detuning of the energy levels leads to an additional rotation about the z axis in the Bloch sphere of the marked and also of neighboring qubits. Moreover, off-resonant shaking of a lattice site can also induce a slight phase shift [18] leading to a general dephasing of the qubits. These effects lead predominantly to additional terms in the Hamiltonian of the form $\hat{W} = \sum_j a_j \hat{\sigma}_z^{(j)}$,

where the Pauli z operator $\sigma_z^{(j)}$ acts on qubit j. If the a_i's are known one can account for the additional z rotations within the quantum calculation. However, one can also cancel these rotations by applying a scheme similar to the refocussing technique well known from NMR quantum control [18]. Suppose an x rotation $\hat{X}_\phi^{(s)} = \exp(i\phi\hat{\sigma}_x^{(s)}/2)$ is to be driven on a qubit at site s. The time 2τ of the operation is chosen such that $\exp(-i\tau a_s \hat{\sigma}_z^{(s)}/2) = 1$. Then, inserting a global π rotation $\hat{X}_\pi^{\text{gl}} = \exp(i\pi/2 \sum_j \hat{\sigma}_x^{(j)})$ before and in the middle of the operation does not perturb the $\hat{X}_\phi^{(s)}$ rotation but all z rotations are cancelled since $\hat{X}_\pi^{\text{gl}}$ has the property that $\hat{X}_\pi^{\text{gl}} e^{-it\hat{W}/\hbar} \hat{X}_\pi^{\text{gl}} e^{-it\hat{W}/\hbar} = 1$.

Together with single-qubit operations, the ability to drive a controlled rotation (CROT) between adjacent lattice sites completes a universal gate set [23]. A CROT rotates one qubit (the target qubit) if and only if another qubit (the control qubit) is in state $|1\rangle$. The strategy to perform this operation between neighboring qubits is to deform the lattice such that a repulsively bound state $\left\|{}^{02}_{00}\right\rangle$ [24] comes into resonance with the state $|00\rangle = \left\|{}^{11}_{00}\right\rangle$. The coupling between the lattice sites leads to an avoided crossing in the energy spectrum (see Fig. 2). If we identify the left qubit with the control qubit, any rotation like that of Eq. (2) on the right target qubit becomes off-resonant and is inhibited iff the control qubit is initially in the excited state ($|0\rangle$).
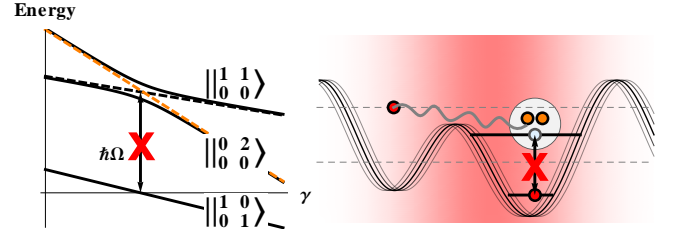

FIG. 2. (Color online) A laser (red shading in right image) is positioned slightly offset from the middle between two lattice sites so that both lattice sites are coupled and the energy of the right lattice site is lower than the one of the left site. At a certain laser intensity the energy of the repulsively bound state $\left\|{}^{02}_{00}\right\rangle$ and the state $\left\|{}^{11}_{00}\right\rangle$ form an avoided crossing (left image). It is now possible to shake the lattice with frequency Ω resonantly to the transition $|10\rangle \leftrightarrow |11\rangle$ ($\left\|{}^{01}_{10}\right\rangle \leftrightarrow \left\|{}^{00}_{11}\right\rangle$) while the transition $|00\rangle \leftrightarrow |01\rangle$ ($\left\|{}^{11}_{00}\right\rangle \leftrightarrow \left\|{}^{10}_{01}\right\rangle$) is off-resonant. This enables rotations on the right target qubit conditioned by the left control qubit.

In order to validate the proposal for single and two-qubit operations by a numerical study a lattice with unit filling described by a Wannier basis of the first three Bloch bands with periodic boundary conditions is considered. It is assumed that the lattice is sufficiently deep so that, as usual within the Bose-Hubbard model, only next-neighbor hopping and onsite interaction need to be considered. For the single-qubit rotation, a system of two lattice sites suffices to estimate the influence of the

operation on the remaining system and vice versa. For studying the two-qubit operation a third site has to be added. The third Bloch band is included to study possible excitations of atoms out of the qubit basis. In the following a lattice depth $V_0 = 2.7\hbar\omega_L = 29.16$ is considered. For this lattice an interaction strength $g = 1.87$ suffices to form a Mott insulator so that all qubit states are eigenstates of the Hamiltonian.

As an example for a single-qubit operation the NOT operation on the right site of a two-well lattice is considered. As stated above the dephasing caused by terms of the form $\hat{W} = a_1\hat{\sigma}_z^{(1)} + a_2\hat{\sigma}_z^{(2)}$ is inhibited by two global $\hat{X}_\pi^{\rm gl}$ rotations. However, the narrow-waist laser can also lead to a weak coupling $b\hat{\sigma}_z^{(1)} \cdot \hat{\sigma}_z^{(2)}$ which can only be cancelled by more complex sequences of refocussing pulses. To suppress this term during the operation the lattice depth V_0 is temporarily enlarged to $V_0 + \delta V_0$ before shining in the narrow-waist laser. Both perturbations are switched on and off adiabatically and are sufficiently small so that couplings to bands above the third Bloch band are negligible. While the perturbations are active $\hat{V}_{\rm sh}$ drives resonantly in the adiabatic basis the rotation $\hat{U} = \exp(i\Omega_R t\hat{\sigma}_x/2)$ on the right site, which for $\Omega_R t = \pi$ is the NOT operation up to a global phase. Fig. 3 shows numerical simulations for the NOT
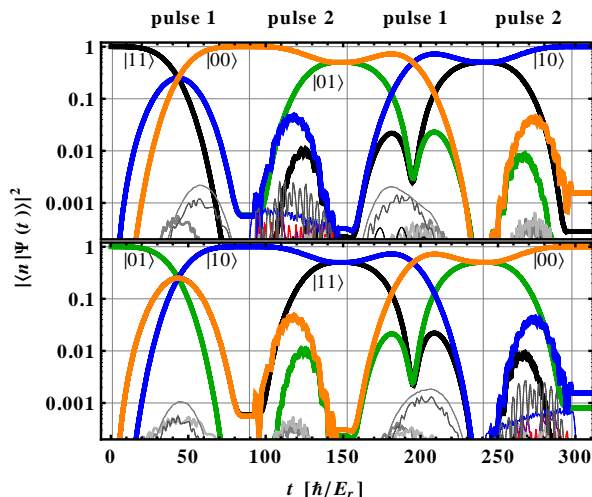

FIG. 3. (Color online) Admixtures of different eigenstates for the initial states $|11\rangle$ and $|01\rangle$ during a NOT operation on the right qubit of a two-well lattice. Pulse 1 drives an $\hat{X}_\pi^{\rm gl}$ rotation. Pulse 2 starts by linearly increasing the lattice depth by $\delta V_0 = 0.17V_0$ during a ramping time of $5.9\hbar/E_r$. Then the Gaussian beam with waist $\sigma = \pi/2$ centered at the site of the target qubit is linearly ramped during a time of $0.4\hbar/E_r$ to the strength $\gamma = 2.62$. After a $\pi/2$ rotation ($\sqrt{\rm NOT}$) on the right qubit driven by shaking the lattice resonantly to the energy difference between $|11\rangle$ and $|10\rangle$, δV_0 and γ are ramped off in reversed order. The simulations show a fidelity of 99.7% for a gate time of $300\hbar/E_r$.

operation including two $\hat{X}_\phi^{\rm gl}$ operations for refocussing.

For the chosen parameter set (see caption of Fig. 3) the influence of the qubit state on the left side is negligible and an average fidelity [25] of 99.7% is reached. Without refocussing (not shown) the fidelity would be only 33.2% due to dephasing.

For the CROT operation a system of three lattice sites is considered. The left site acts as the control qubit of an $\hat{X}_\pi^{(2)}$ rotation on the central target qubit. Up to a local phase this operation is equivalent to a controlled-NOT operation. Due to the periodic boundary conditions the right site is coupled to the control and the target qubit. Example results and parameters of the numerical simulations of the CROT are shown in Fig. 4. For a gate time of $400\hbar/E_r$ an average fidelity of 99.4% is reached. For the evaluation of the fidelity the individual z rotations and those z rotations coupled to the control qubit are neglected. This is possible since equipped with the global $\hat{X}_\pi^{\rm gl}$ and local NOT operations these z rotation can be easily cancelled by using a refocusing scheme. Opposing to the NOT operation an important source of infidelity of the CROT stems from the leakage to states out of the qubit basis. Averaged over the computational basis the leakage probability after the operation is 0.27%. To diminish this one can either use techniques of leakage elimination [26] or one has to choose a deeper lattice. This leads to weaker coupling between the lattice sites and thus to longer gate times. Increasing, e.g., the lattice depth V_0 from $2.7\hbar\omega_L$ to $2.8\hbar\omega_L$ and the gate time to $540\hbar/E_r$ reduces the leakage probability to 0.15% and increases the fidelity by another 0.06%.

Independently of the chosen lattice depth, the time scale $\hbar/E_r$ is a crucial system parameter for the speed and accuracy of the manipulations. In general a large recoil energy $E_r = \hbar^2 k^2/2m$ allows shorter time scales. For example, the NOT operation for a ^{87}Rb system in a $d = 500$ nm OL ($E_r = 1.5 \times 10^{-30}$ J) lasts 21 ms while the same operation would take 0.6 ms for ^{7}Li in a $d = 300$ nm lattice ($E_r = 5.2 \times 10^{-29}$ J).

In order for the operations to be robust any relative energy shift of the manipulated qubit states by some external perturbation must be small compared to the energy scale of the Rabi oscillations $\hbar\Omega_R$ which in our case is about $0.1\,E_r$. Since the energy differences are mainly influenced by the lattice potential itself, its uncontrolled perturbation can severely reduce the fidelity of the operation. Considering the CROT operation, which is more sensitive to perturbations than single-qubit operations, only a lattice laser intensity which is controlled on the 10^{-4} level leads to negligible fidelity reduction (see Tab. I). On the other hand, perturbations of other parameters such as the intensity of the gaussian laser beam or the interaction strength are much less severe.

The last important ingredient for quantum computation is the possibility to read out qubit states with high fidelity. This can be done by removing atoms in the excited state $|0\rangle$ from the lattice and determining subse-

TABLE I. Average fidelity of the CROT operation presented in Fig. 4 for uncontrolled errors of the interaction strength g, the strength of the gaussian laser γ, and the lattice depth V_0.

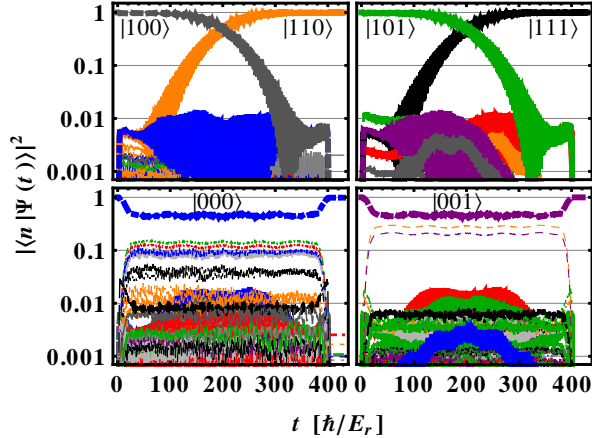| Parameter	g		γ		V_0		
Error	0.1%	1%	0.1%	1%	0.01%	0.1%	1%
Fidelity	99.4%	98.1%	98.9%	97.3%	99.2%	90.9%	31.4%

FIG. 4. (Color online) Admixtures of different eigenstates for different initial states during a CROT on the left control qubit at $x = 0$ and the central target qubit at $x = \pi$. The Gaussian beam with waist $\sigma = \pi/2$ at $x_0 = 0.6\pi$ is linearly ramped to a strength of $\gamma = 0.224$ during a time of $2\hbar/E_r$. After waiting for $12\hbar/E_r$ the beam is linearly ramped for $16\hbar/E_r$ to the avoided crossing with the repulsively bound state at $\gamma = 0.204$. After shaking the lattice resonantly to the energy difference between $|111\rangle$ and $|101\rangle$ the gaussian beam is switched off in reversed order. For a gate time of $400\hbar/E_r$ a fidelity of 99.4% is reached (see text).

quently the atom distribution of the remaining atoms by fluorescence imaging with single-site resolution. The removal of excited atoms is related to an evaporative cooling of the system and corresponding strategies may be applied. One method is to accelerate the lattice in x direction. For sufficiently deep lattices the large gap between the first and second Bloch bands inhibits Landau-Zener transitions such that atoms in the ground state $|1\rangle$ are dragged by the lattice. However, atoms in state $|0\rangle$ may tunnel to higher Bloch bands and eventually leave the lattice [27, 28]. The tunneling can be enhanced by first transferring atoms in state $|0\rangle$ to a higher Bloch band. As shown in Fig. 5 for the exemplary lattice depth of $V_0 = 2.7\hbar\omega_L$ one can drive transitions from the 2nd to the high-lying 5th Bloch band by means of shaking the lattice with frequency $\Omega_{2,5}$ while transitions from the first Bloch band are inhibited due to a band gap. In the 5th Bloch band the atoms are quasi-free and leave the lattice even during slow accelerations. Lately, a closely related scheme of a state-dependent removal of atoms from an optical lattice has been used experimentally for cool-

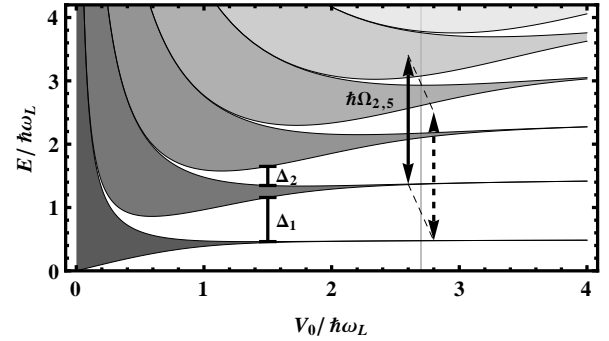ing a quantum gas [29] supporting the practicability of vibrationally encoded qubits and the proposed read-out scheme.

FIG. 5. Energy widths of the Bloch bands as a function of the lattice depth. For shallow lattices the band gap Δ_2 is much smaller than Δ_1. When moving the lattice this allows for Landau-Zener transitions out of the 2nd band while atoms in the 1st band are dragged by the lattice. At $V_0 = 2.7\hbar\omega$ one may drive a transition from the 2nd to the 5th Bloch band with energy difference $\hbar\Omega_{2,5}$ while a transition from the first Bloch band is forbidden by a band gap.

In conclusion, a scheme for quantum computation with Bosons in 1d optical lattices was presented. The qubits are encoded in the spacial atomic wave function which suppresses decoherence due to fluctuating magnetic fields. It was shown that by shaking the lattice one may drive single and controlled qubit rotations and how qubit dephasing can be prevented by using refocussing pulses. The qubit readout can be performed by removing atoms in excited states from the lattice and determining the atom distribution by fluorescence imaging. For gate times on the order of milliseconds fidelities above 99% can be reached. We believe that gate times and fidelities can be further improved, e.g., by using optimal control. It would be interesting to extend the approach to a 2d OL in order to reduce the number of needed swap operations. However, considering ^{7}Li atoms in a $d = 300\,\text{nm}$ lattice, already within the 1d approach a factorization of 15 would be feasible within about 50 ms with about 20 ms needed for swapping operations.

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